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Electron Capture from Atomic Nitrogen by Protons

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Electron Capture from Atomic Nitrogen by Protons

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The total Oppenheimer-Brinkman-Kramers (OBK) cross sections for $1s$-, $2s$-, and $2p$-orbital electron capture from atomic nitrogen by protons are adjusted to correspond to capture from N_2 by deuterons, and are compared with recent measurements of Berkner *et al*. Calculated cross sections for $1s$ capture are dominant above 3 MeV, and the total OBK cross section still exceeds the measured cross section at the deuteron energy of 21.5 MeV.

RECENTLY published measurements of cross sections for electron capture from N_2 by deuterons differ markedly from the OBK (Oppenheimer-Brinkman-Kramers) cross sections for electron capture from N by protons when expressed as cross sections per gas molecule at the appropriate impact energy for deuterons.[1] One of the chief sources of the disagreement in this comparison originates from using calculated cross sections for only p-orbital capture at impact energies where capture from inner subshells is dominant.[2]

The importance of $1s$- and $2s$-orbital capture at high impact energies was emphasized in I, but only estimates of these cross sections could be given since the wave functions for the atomic ions, $N^+(^5S,^3S)$, configurations $(1s)^2 2s(2p)^3$ and $1s(2s)^2(2p)^3$, were not available during the time that the calculations were effected. Since wave functions have become available,[3] OBK cross sections for $2s$-orbital capture have been computed and published.[4] Although wave functions for the configuration $1s(2s)^2(2p)^3$ have not been published, the atomic orbitals for the ion Ne^+, configurations $1s(2s)^2(2p)^6$ and $(1s)^2 2s(2p)^6$, are given in a recent paper.[5] A comparison of the orbital functions for these two configurations of Ne^+ shows that the two sets of $1s$ and $2s$ parameters differ very little. With this in mind, it is assumed that not much error in the OBK cross sections for $1s$ capture result from using Roothaan[3] atomic orbitals of $(1s)^2 2s(2p)^3$, $N^+(^5S,^3S)$, to represent the corresponding term values of $1s(2s)^2(2p)^3$. (This is a very special application of the wave functions, and is not supposed to imply the validity of such an approximation for other purposes.)

This approximation has been used to compute cross sections for $1s$ capture, impact energies ≥ 1 MeV; moreover, the energy range of the cross sections for $2s$ capture[4] has been extended to 100 MeV. The cross sections are expressed as a function of the impact energy of the proton in the frame of reference where the atomic target is initially at rest. Perhaps the most notable distinction of these OBK cross sections is the dominance of $1s$-orbital capture for impact energies exceeding 3 MeV. These cross sections pertain to capture into the $1s$ state of atomic hydrogen only, and the n^{-3} rule is used to sum the cross sections into all s states of hydrogen.[6] As for the contributions of simultaneous charge transfer and excitation, previous calculations for helium suggest that these processes can be neglected with small error.[7] The sum of the OBK cross sections for $1s$-, $2s$-, and $2p$-orbital capture from $N(^4S)$ into all s states of the hydrogen atom leaving the residual ions $N^+[^3P;(1s)^2(2s)^2(2p)^2]$, $N^+[^3S,^5S;(1s)^2 2s(2p)^3]$, and $N^+[^3S,^5S;1s(2s)^2(2p)^3]$ have been multiplied by 2, and are plotted in Fig. 1.

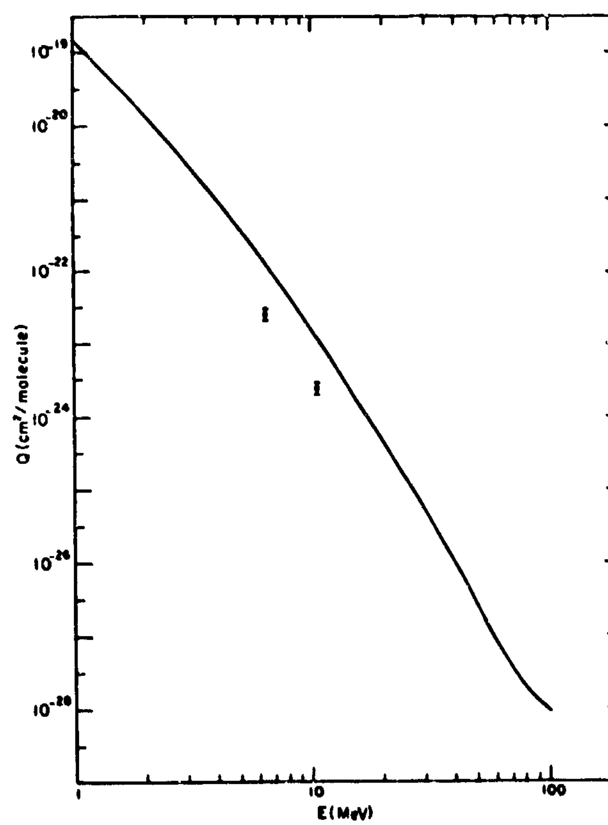

FIG. 1. Electron-capture cross sections per N_2 molecule. E is the impact energy of the proton in MeV. Closed circles with error bar represent experimental values taken from Table I of Berkner *et al.* Solid curve represents the sum of the OBK cross sections for atomic nitrogen multiplied by 2. (See text for the processes represented.)

[1] K. H. Berkner, S. N. Kaplan, G. A. Paulikas, and R. V. Pyle, Phys. Rev. 140, A729 (1965).
[2] R. A. Mapleton, Phys. Rev. 130, 1829 (1963). This is referred to as I.
[3] C. C. J. Roothaan and P. S. Kelley, Phys. Rev. 131, 1177 (1963).
[4] R. A. Mapleton, Proc. Phys. Soc. (London) 85, 1109 (1965).
[5] P. S. Bagus, Phys. Rev. 139, A619 (1965).
[6] J. R. Oppenheimer, Phys. Rev. 31, 349 (1928); J. D. Jackson and H. Schiff, *ibid.* 89, 359 (1953).
[7] R. A. Mapleton, Phys. Rev. 122, 528 (1961).

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It is seen that the two experimental values of Berkner, *et al.* are less than the corresponding OBK values, which fact suggests that the asymptotic energy region may not yet be reached. Of course, it is not known whether OBK cross sections are the asymptotic values of a correct theory, and at what energy the onset of the asymptotic value would occur. Little is also known how well electron capture from N_2 can be described in terms of N atoms[8] (factor of 2) or how much the present OBK values would be altered by a recalculation with improved wave functions. In the author's opinion, it is very difficult to decide theoretically what the asymptotic cross section is for a target as complicated as N_2.

An atomic system much more tractable to theoretical analysis is helium, and the energy range of the OBK calculations[9] using the 6-parameter helium wave function have also been extended to 100 MeV. The OBK cross sections for capture from He, N, and O, described in this paper, can be obtained from the author.

Gratitude is expressed to Professor A. Dalgarno for informing the author of these measurements.

[8] T. F. Tuan and E. Gerjuoy, Phys. Rev. 117, 756 (1960).

[9] R. A. Mapleton, Phys. Rev. 130, 1839 (1963).

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13. ABSTRACT

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